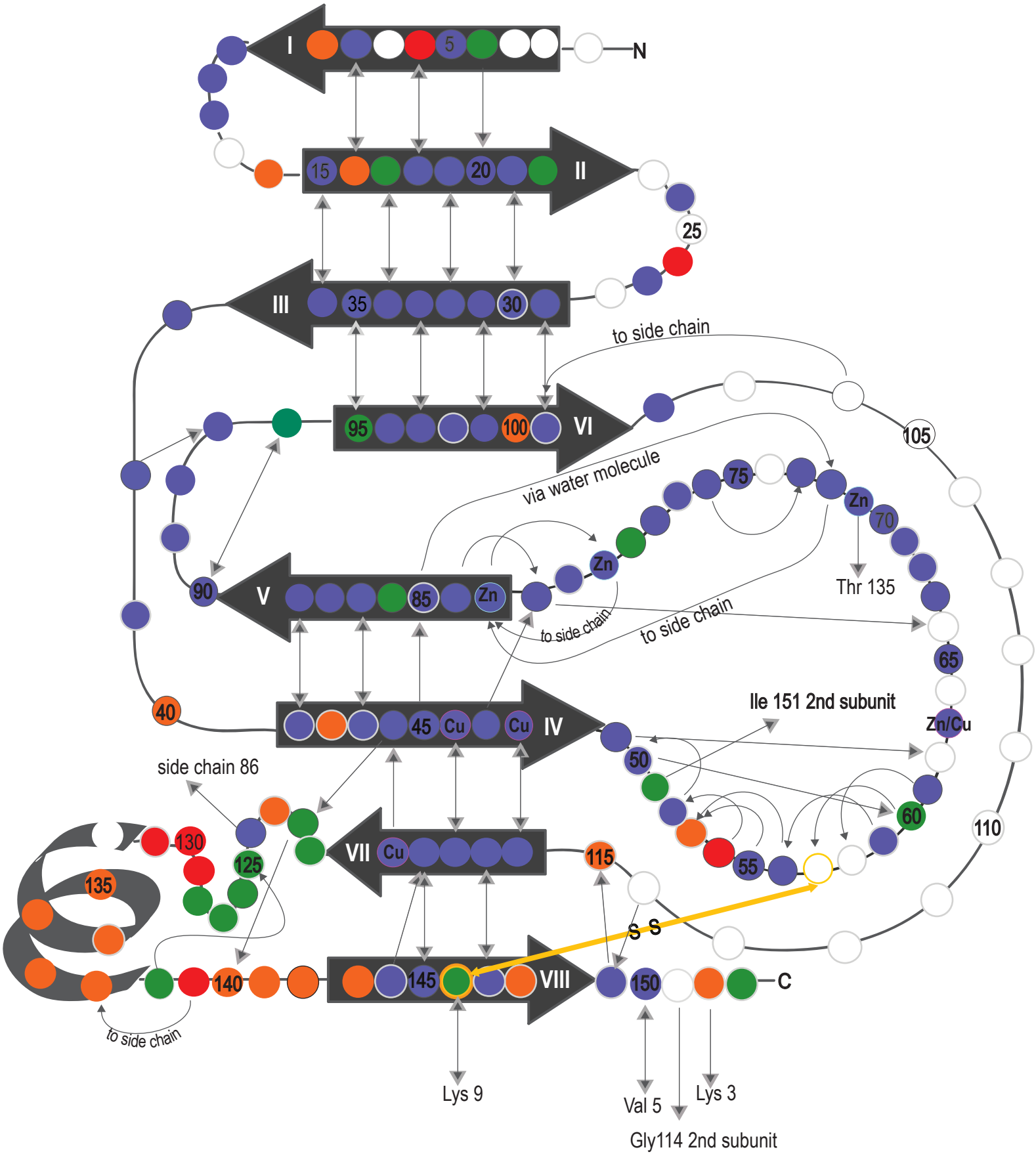
I
5
N
15
20
II
25
III
35
30
to side chain
95
100
VI
105
via water molecule
75
Zn
70
90
V
85
Zn
Zn
Thr 135
to side chain
to side chain
65
40
45
Cu
Cu
IV
Ile 151 2nd subunit
Zn/Cu
side chain 86
50
60
110
130
125
VII
Cu
115
135
55
S S
140
145
VIII
150
C
to side chain
Lys 9
Val 5
Lys 3
Gly114 2nd subunit

Supplementary Figure 1: Schematic of one CuZnSOD subunit showing the differences in exchange patterns for the I113T variant at 37°C compared to 25°C. Amide protons, which exchange up to one order of magnitude faster at 37°C than at 25°C, are colored in blue. Amide protons, which exchange faster than one order of magnitude, are colored green. Amide protons, which exchange faster than two orders of magnitude, are colored orange and amide protons, which exchange faster than three orders of magnitude, are colored red. Amino acids that are not assigned (prolines included) due to overlap and weak or missing peaks are colored white. Copper and zinc binding sites are labeled with Cu and Zn, respectively. The black numbered arrows illustrate the eight β-sheets, and the gray arrows between the amino acids indicate hydrogen bonds in the secondary structure as determined from the crystal structure (PDB accession no. 2C9V) pointing from H to O.

Table 1: Supplementary Table 1: H/D exchange parameters for I113T at 37°C

Residue	$k_{ex}(min^{-1})$	$t_{1/2}(min)$	$k_{ch}(min^{-1})$	K_{op}	$\Delta G_{op}(kcalmol^{-1}l^{-1})$
Ala1	n/a	n/a	n/a	n/a	n/a
Thr2	n/a	n/a	n/a	n/a	n/a
Lys3	n/a	n/a	n/a	n/a	n/a
Ala4	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$6.7 \cdot 10^{3}$	$6.0 \cdot 10^{-6} < K_{op} < 9.0 \cdot 10^{-3}$	$2.9 < \Delta G_{op} < 7.4$
Val5	$3.7 \cdot 10^{-5}$	$1.9 \cdot 10^{4}$	$1.0 \cdot 10^{3}$	$3.7 \cdot 10^{-8}$	10.5
Cys6	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$3.7 \cdot 10^{3}$	$1.1 \cdot 10^{-5} < K_{op} < 1.6 \cdot 10^{-2}$	$2.5 < \Delta G_{op} < 7.0$
Val7	n/a	n/a	n/a	n/a	n/a
Leu8	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$1.0 \cdot 10^{3}$	$< 3.6 \cdot 10^{-8}$	> 10.6
Lys9	$3.4 \cdot 10^{-2}$	$2.0 \cdot 10^{1}$	$2.9 \cdot 10^{3}$	$1.2 \cdot 10^{-5}$	7.0
Gly10	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.3 \cdot 10^{4}$	$3.2 \cdot 10^{-6} < K_{op} < 4.8 \cdot 10^{-3}$	$3.3 < \Delta G_{op} < 7.8$
Asp11	$1.8 \cdot 10^{2}$	$3.9 \cdot 10^{-3}$	$3.8 \cdot 10^{3}$	$4.7 \cdot 10^{-2}$	1.9
Gly12	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$6.3 \cdot 10^{3}$	$6.4 \cdot 10^{-6} < K_{op} < 9.6 \cdot 10^{-3}$	$2.9 < \Delta G_{op} < 7.4$
Pro13	n/a	n/a	n/a	n/a	n/a
Val14	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$4.0 \cdot 10^{3}$	$9.9 \cdot 10^{-6} < K_{op} < 1.5 \cdot 10^{-2}$	$2.6 < \Delta G_{op} < 7.1$
Gln15	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$4.2 \cdot 10^{3}$	$9.5 \cdot 10^{-6} < K_{op} < 1.4 \cdot 10^{-2}$	$2.6 < \Delta G_{op} < 7.1$
Gly16	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.5 \cdot 10^{4}$	$2.7 \cdot 10^{-6} < K_{op} < 4.0 \cdot 10^{-3}$	$3.4 < \Delta G_{op} < 7.9$
Val17	$1.1 \cdot 10^{-2}$	$5.8 \cdot 10^{3}$	$1.4 \cdot 10^{3}$	$8.5 \cdot 10^{-6}$	7.2
Ile18	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$5.6 \cdot 10^{2}$	$< 6.4 \cdot 10^{-8}$	> 10.2
Asn19	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$9.2 \cdot 10^{3}$	$< 3.9 \cdot 10^{-9}$	> 11.9
Phe20	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$6.1 \cdot 10^{3}$	$< 5.9 \cdot 10^{-9}$	> 11.7
Glu21	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$1.8 \cdot 10^{3}$	$< 2.0 \cdot 10^{-8}$	> 10.9
Gln22	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$4.1 \cdot 10^{3}$	$9.7 \cdot 10^{-6} < K_{op} < 1.4 \cdot 10^{-2}$	$2.6 < \Delta G_{op} < 7.1$
Lys23	n/a	n/a	n/a	n/a	n/a
Glu24	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$2.1 \cdot 10^{3}$	$1.9 \cdot 10^{-5} < K_{op} < 2.9 \cdot 10^{-2}$	$2.2 < \Delta G_{op} < 6.7$
Ser25	n/a	n/a	n/a	n/a	n/a
Asn26	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$3.1 \cdot 10^{4}$	$1.3 \cdot 10^{-6} < K_{op} < 1.9 \cdot 10^{-3}$	$3.9 < \Delta G_{op} < 8.4$
Gly27	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$2.0 \cdot 10^{4}$	$2.0 \cdot 10^{-6} < K_{op} < 3.0 \cdot 10^{-3}$	$3.6 < \Delta G_{op} < 8.0$
Pro28	n/a	n/a	n/a	n/a	n/a
Val29	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$4.0 \cdot 10^{3}$	$< 9.0 \cdot 10^{-9}$	> 11.4
Lys30	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$3.4 \cdot 10^{3}$	$< 1.1 \cdot 10^{-8}$	> 11.3
Val31	$4.5 \cdot 10^{-4}$	$1.5 \cdot 10^{3}$	$1.3 \cdot 10^{3}$	$3.4 \cdot 10^{-7}$	9.2
Trp32	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$1.4 \cdot 10^{3}$	$< 2.6 \cdot 10^{-8}$	> 10.8
Gly33	$4.7 \cdot 10^{-4}$	$1.5 \cdot 10^{3}$	$7.3 \cdot 10^{3}$	$6.4 \cdot 10^{-8}$	10.2
Ser34	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.8 \cdot 10^{4}$	$2.3 \cdot 10^{-6} < K_{op} < 3.4 \cdot 10^{-3}$	$3.5 < \Delta G_{op} < 8.0$
Ile35	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$1.9 \cdot 10^{3}$	$< 1.9 \cdot 10^{-8}$	> 10.9
Lys36	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$2.7 \cdot 10^{3}$	$< 1.3 \cdot 10^{-8}$	> 11.2
Gly37	$2.0 \cdot 10^{-2}$	$3.4 \cdot 10^{1}$	$1.3 \cdot 10^{4}$	$1.6 \cdot 10^{-6}$	8.2
Leu38	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$2.0 \cdot 10^{3}$	$< 1.8 \cdot 10^{-8}$	> 11.0
Thr39	$5.5 \cdot 10^{-4}$	$1.3 \cdot 10^{3}$	$2.7 \cdot 10^{3}$	$2.1 \cdot 10^{-7}$	9.5
Glu40	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$2.5 \cdot 10^{3}$	$1.6 \cdot 10^{-5} < K_{op} < 2.4 \cdot 10^{-2}$	$2.3 < \Delta G_{op} < 6.8$
Gly41	$4.4 \cdot 10^{-3}$	$1.6 \cdot 10^{2}$	$6.7 \cdot 10^{3}$	$6.5 \cdot 10^{-7}$	8.8
Leu42	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$2.0 \cdot 10^{3}$	$2.0 \cdot 10^{-5} < K_{op} < 3.0 \cdot 10^{-2}$	$2.2 < \Delta G_{op} < 6.7$
His43	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$2.0 \cdot 10^{4}$	$< 1.8 \cdot 10^{-9}$	> 12.4
Gly44	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$6.4 \cdot 10^{4}$	$< 5.6 \cdot 10^{-10}$	> 13.1
Phe45	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$4.3 \cdot 10^{3}$	$< 8.4 \cdot 10^{-9}$	> 11.4
His46	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$3.7 \cdot 10^{4}$	$< 9.7 \cdot 10^{-10}$	> 12.8
Val47	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$2.0 \cdot 10^{4}$	$< 1.8 \cdot 10^{-9}$	> 12.4
His48	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$2.3 \cdot 10^{4}$	$1.7 \cdot 10^{-6} < K_{op} < 2.6 \cdot 10^{-3}$	$3.7 < \Delta G_{op} < 8.2$
Glu49	$2.3 \cdot 10^{2}$	$3.0 \cdot 10^{-3}$	$1.1 \cdot 10^{4}$	$2.2 \cdot 10^{-2}$	2.4
Phe50	$7.1 \cdot 10^{1}$	$9.8 \cdot 10^{-3}$	$2.0 \cdot 10^{3}$	$3.4 \cdot 10^{-2}$	2.1
Gly51	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.1 \cdot 10^{4}$	$3.7 \cdot 10^{-6} < K_{op} < 5.5 \cdot 10^{-3}$	$3.2 < \Delta G_{op} < 7.7$
Asp52	$3.6 \cdot 10^{-3}$	$1.9 \cdot 10^{2}$	$3.8 \cdot 10^{3}$	$9.6 \cdot 10^{-7}$	8.5
Asn53	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.0 \cdot 10^{4}$	$3.9 \cdot 10^{-6} < K_{op} < 5.8 \cdot 10^{-3}$	$3.2 < \Delta G_{op} < 7.7$
Thr54	$3.7 \cdot 10^{2}$	$1.9 \cdot 10^{-3}$	$9.0 \cdot 10^{3}$	$4.1 \cdot 10^{-2}$	1.9
Ala55	$8.4 \cdot 10^{1}$	$8.3 \cdot 10^{-3}$	$8.0 \cdot 10^{3}$	$1.0 \cdot 10^{-2}$	2.8
Gly56	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$9.5 \cdot 10^{3}$	$4.2 \cdot 10^{-6} < K_{op} < 6.3 \cdot 10^{-3}$	$3.1 < \Delta G_{op} < 7.6$
Cys57	n/a	n/a	n/a	n/a	n/a
Thr58	n/a	n/a	n/a	n/a	n/a
Ser59	$2.0 \cdot 10^{2}$	$3.5 \cdot 10^{-3}$	$1.9 \cdot 10^{4}$	$1.0 \cdot 10^{-2}$	2.8
Ala60	$1.7 \cdot 10^{-2}$	$4.1 \cdot 10^{1}$	$1.0 \cdot 10^{4}$	$1.7 \cdot 10^{-6}$	7.9
Gly61	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$9.5 \cdot 10^{3}$	$4.2 \cdot 10^{-6} < K_{op} < 6.3 \cdot 10^{-3}$	$3.1 < \Delta G_{op} < 7.6$

Residue	$k_{ex}(min^{-1})$	$t_{1/2}(min)$	$k_{ch}(min^{-1})$	K_{op}	$\Delta G_{op}(kcalmol^{-1}l^{-1})$
Pro62	n/a	n/a	n/a	n/a	n/a
His63	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.3 \cdot 10^{5}$	$3.1 \cdot 10^{-7} < K_{op} < 4.7 \cdot 10^{-4}$	$4.7 < \Delta G_{op} < 9.2$
Phe64	n/a	n/a	$2.0 \cdot 10^{4}$	n/a	n/a
Asn65	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.8 \cdot 10^{4}$	$2.2 \cdot 10^{-6} < K_{op} < 3.3 \cdot 10^{-3}$	$3.5 < \Delta G_{op} < 8.0$
Pro66	n/a	n/a	n/a	n/a	n/a
Leu67	$3.7 \cdot 10^{2}$	$1.9 \cdot 10^{-3}$	$5.3 \cdot 10^{3}$	$6.9 \cdot 10^{-2}$	1.6
Ser68	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$7.3 \cdot 10^{3}$	$5.4 \cdot 10^{-6} < K_{op} < 8.2 \cdot 10^{-3}$	$3.0 < \Delta G_{op} < 7.5$
Arg69	$9.5 \cdot 10^{1}$	$7.3 \cdot 10^{-3}$	$1.2 \cdot 10^{4}$	$7.8 \cdot 10^{-3}$	3.0
Lys70	$2.5 \cdot 10^{2}$	$2.8 \cdot 10^{-3}$	$7.7 \cdot 10^{3}$	$3.2 \cdot 10^{-2}$	2.1
His71	$4.1 \cdot 10^{-4}$	$1.7 \cdot 10^{3}$	$4.2 \cdot 10^{4}$	$9.7 \cdot 10^{-9}$	11.4
Gly72	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$6.4 \cdot 10^{4}$	$< 5.6 \cdot 10^{-10}$	> 13.1
Gly73	$7.8 \cdot 10^{-5}$	$8.9 \cdot 10^{3}$	$1.4 \cdot 10^{4}$	$5.6 \cdot 10^{-9}$	11.7
Pro74	n/a	n/a	n/a	n/a	n/a
Lys75	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.8 \cdot 10^{4}$	$2.2 \cdot 10^{-6} < K_{op} < 3.3 \cdot 10^{-3}$	$3.5 < \Delta G_{op} < 8.0$
Asp76	$1.2 \cdot 10^{-2}$	$5.8 \cdot 10^{1}$	$3.4 \cdot 10^{3}$	$3.6 \cdot 10^{-6}$	7.7
Glu77	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.0 \cdot 10^{3}$	$3.9 \cdot 10^{-5} < K_{op} < 5.8 \cdot 10^{-2}$	$1.8 < \Delta G_{op} < 6.3$
Glu78	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.1 \cdot 10^{3}$	$3.6 \cdot 10^{-5} < K_{op} < 5.4 \cdot 10^{-2}$	$1.8 < \Delta G_{op} < 6.3$
Arg79	$1.9 \cdot 10^{-2}$	$3.7 \cdot 10^{1}$	$4.3 \cdot 10^{3}$	$4.3 \cdot 10^{-6}$	7.6
His80	$1.6 \cdot 10^{2}$	$4.4 \cdot 10^{-3}$	$5.3 \cdot 10^{4}$	$3.0 \cdot 10^{-3}$	3.6
Val81	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$6.8 \cdot 10^{3}$	$5.8 \cdot 10^{-6} < K_{op} < 8.8 \cdot 10^{-3}$	$2.9 < \Delta G_{op} < 7.4$
Gly82	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$6.8 \cdot 10^{3}$	$5.8 \cdot 10^{-6} < K_{op} < 8.8 \cdot 10^{-3}$	$2.9 < \Delta G_{op} < 7.4$
Asp83	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$3.8 \cdot 10^{3}$	$< 9.5 \cdot 10^{-9}$	> 11.4
Leu84	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$8.9 \cdot 10^{2}$	$< 4.0 \cdot 10^{-8}$	> 10.5
Gly85	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$5.8 \cdot 10^{3}$	$< 6.2 \cdot 10^{-9}$	> 11.6
Asn86	$1.2 \cdot 10^{-2}$	$5.8 \cdot 10^{1}$	$2.3 \cdot 10^{4}$	$5.2 \cdot 10^{-7}$	8.9
Val87	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$2.1 \cdot 10^{3}$	$< 1.7 \cdot 10^{-8}$	> 11.0
Thr88	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$3.1 \cdot 10^{3}$	$1.3 \cdot 10^{-5} < K_{op} < 1.9 \cdot 10^{-2}$	$2.4 < \Delta G_{op} < 6.9$
Ala89	$4.3 \cdot 10^{-5}$	$1.6 \cdot 10^{4}$	$8.1 \cdot 10^{3}$	$5.4 \cdot 10^{-9}$	11.7
Asp90	$6.8 \cdot 10^{1}$	$1.0 \cdot 10^{-2}$	$2.6 \cdot 10^{3}$	$2.7 \cdot 10^{-2}$	2.2
Lys91	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$3.1 \cdot 10^{3}$	$1.3 \cdot 10^{-5} < K_{op} < 2.0 \cdot 10^{-2}$	$2.4 < \Delta G_{op} < 6.9$
Asp92	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$3.4 \cdot 10^{3}$	$1.2 \cdot 10^{-5} < K_{op} < 1.8 \cdot 10^{-2}$	$2.5 < \Delta G_{op} < 7.0$
Gly93	$4.5 \cdot 10^{-3}$	$1.5 \cdot 10^{2}$	$6.3 \cdot 10^{3}$	$7.2 \cdot 10^{-7}$	8.7
Val94	$1.5 \cdot 10^{-3}$	$4.5 \cdot 10^{2}$	$1.5 \cdot 10^{3}$	$1.0 \cdot 10^{-6}$	8.5
Ala95	$2.2 \cdot 10^{-4}$	$3.0 \cdot 10^{3}$	$3.7 \cdot 10^{3}$	$6.3 \cdot 10^{-8}$	10.2
Asp96	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$2.6 \cdot 10^{3}$	$1.6 \cdot 10^{-5} < K_{op} < 2.4 \cdot 10^{-2}$	$2.3 < \Delta G_{op} < 6.8$
Val97	$1.3 \cdot 10^{-4}$	$5.5 \cdot 10^{3}$	$6.7 \cdot 10^{2}$	$1.9 \cdot 10^{-7}$	9.5
Ser98	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$8.7 \cdot 10^{3}$	$4.6 \cdot 10^{-6} < K_{op} < 7.0 \cdot 10^{-3}$	$3.1 < \Delta G_{op} < 7.6$
Ile99	$1.1 \cdot 10^{-4}$	$6.2 \cdot 10^{3}$	$1.9 \cdot 10^{3}$	$5.9 \cdot 10^{-8}$	10.2
Glu100	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$9.2 \cdot 10^{2}$	$4.3 \cdot 10^{-5} < K_{op} < 6.5 \cdot 10^{-2}$	$1.7 < \Delta G_{op} < 6.2$
Asp101	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.8 \cdot 10^{3}$	$2.2 \cdot 10^{-5} < K_{op} < 3.3 \cdot 10^{-2}$	$2.1 < \Delta G_{op} < 6.6$
Ser102	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$7.9 \cdot 10^{3}$	$5.1 \cdot 10^{-6} < K_{op} < 7.6 \cdot 10^{-3}$	$3.0 < \Delta G_{op} < 7.5$
Val103	n/a	n/a	n/a	n/a	n/a
Ile104	n/a	n/a	n/a	n/a	n/a
Ser105	n/a	n/a	n/a	n/a	n/a
Leu106	n/a	n/a	n/a	n/a	n/a
Ser107	n/a	n/a	n/a	n/a	n/a
Gly108	n/a	n/a	n/a	n/a	n/a
Asp109	n/a	n/a	n/a	n/a	n/a
His110	n/a	n/a	n/a	n/a	n/a
Cys111	n/a	n/a	n/a	n/a	n/a
Ile112	n/a	n/a	n/a	n/a	n/a
Thr113	n/a	n/a	n/a	n/a	n/a
Gly114	n/a	n/a	n/a	n/a	n/a
Arg115	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$9.0 \cdot 10^{3}$	$4.4 \cdot 10^{-6} < K_{op} < 6.6 \cdot 10^{-3}$	$3.1 < \Delta G_{op} < 7.6$
Thr116	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$7.2 \cdot 10^{3}$	$< 5.0 \cdot 10^{-9}$	> 11.8
Leu117	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$2.1 \cdot 10^{3}$	$< 1.7 \cdot 10^{-8}$	> 11.0
Val118	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$6.2 \cdot 10^{2}$	$< 5.8 \cdot 10^{-8}$	> 10.3
Val119	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$7.3 \cdot 10^{2}$	$< 4.9 \cdot 10^{-8}$	> 10.4
His120	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$2.3 \cdot 10^{4}$	$< 1.6 \cdot 10^{-9}$	> 12.5
Glu121	$1.9 \cdot 10^{-4}$	$3.6 \cdot 10^{3}$	$1.1 \cdot 10^{4}$	$1.8 \cdot 10^{-8}$	11.0
Lys122	$4.3 \cdot 10^{-5}$	$1.6 \cdot 10^{4}$	$3.3 \cdot 10^{3}$	$1.3 \cdot 10^{-8}$	11.2
Ala123	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$6.7 \cdot 10^{3}$	$6.0 \cdot 10^{-6} < K_{op} < 9.0 \cdot 10^{-3}$	$2.9 < \Delta G_{op} < 7.4$
Asp124	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$2.6 \cdot 10^{3}$	$< 1.4 \cdot 10^{-8}$	> 11.1
Asp125	$2.6 \cdot 10^{-4}$	$2.7 \cdot 10^{3}$	$1.7 \cdot 10^{3}$	$1.5 \cdot 10^{-7}$	9.7
Leu126	$6.3 \cdot 10^{-5}$	$1.1 \cdot 10^{4}$	$8.9 \cdot 10^{2}$	$7.1 \cdot 10^{-8}$	10.1

Residue	$k_{ex}(min^{-1})$	$t_{1/2}(min)$	$k_{ch}(min^{-1})$	K_{op}	$\Delta G_{op}(kcalmol^{-1}l^{-1})$
Gly127	$2.5 \cdot 10^{-4}$	$2.8 \cdot 10^{3}$	$5.8 \cdot 10^{3}$	$4.2 \cdot 10^{-8}$	10.5
Lys128	$2.5 \cdot 10^{-3}$	$2.8 \cdot 10^{2}$	$6.9 \cdot 10^{3}$	$3.6 \cdot 10^{-7}$	9.1
Gly129	$2.8 \cdot 10^{2}$	$2.5 \cdot 10^{-3}$	$1.2 \cdot 10^{4}$	$2.2 \cdot 10^{-2}$	2.3
Gly130	$6.6 \cdot 10^{1}$	$1.0 \cdot 10^{-2}$	$1.4 \cdot 10^{4}$	$4.7 \cdot 10^{-3}$	3.3
Asn131	$1.0 \cdot 10^{2}$	$6.9 \cdot 10^{-3}$	$2.3 \cdot 10^{4}$	$4.3 \cdot 10^{-3}$	3.4
Glu132	n/a	n/a	n/a	n/a	n/a
Glu133	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.1 \cdot 10^{3}$	$3.6 \cdot 10^{-5} < K_{op} < 5.4 \cdot 10^{-2}$	$1.8 < \Delta G_{op} < 6.3$
Ser134	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$8.4 \cdot 10^{3}$	$4.7 \cdot 10^{-6} < K_{op} < 7.1 \cdot 10^{-3}$	$3.0 < \Delta G_{op} < 7.5$
Thr135	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$8.6 \cdot 10^{3}$	$4.6 \cdot 10^{-6} < K_{op} < 7.0 \cdot 10^{-3}$	$3.1 < \Delta G_{op} < 7.6$
Lys136	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$7.3 \cdot 10^{3}$	$5.5 \cdot 10^{-6} < K_{op} < 8.2 \cdot 10^{-3}$	$3.0 < \Delta G_{op} < 7.5$
Thr137	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$5.7 \cdot 10^{3}$	$7.0 \cdot 10^{-6} < K_{op} < 1.1 \cdot 10^{-2}$	$2.8 < \Delta G_{op} < 7.3$
Gly138	$8.7 \cdot 10^{-3}$	$7.9 \cdot 10^{1}$	$1.5 \cdot 10^{4}$	$5.8 \cdot 10^{-7}$	8.8
Asn139	$7.9 \cdot 10^{1}$	$8.8 \cdot 10^{-3}$	$2.3 \cdot 10^{4}$	$3.4 \cdot 10^{-3}$	3.5
Ala140	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.1 \cdot 10^{4}$	$3.8 \cdot 10^{-6} < K_{op} < 5.7 \cdot 10^{-3}$	$3.2 < \Delta G_{op} < 7.7$
Gly141	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$9.5 \cdot 10^{3}$	$4.2 \cdot 10^{-6} < K_{op} < 6.3 \cdot 10^{-3}$	$3.1 < \Delta G_{op} < 7.6$
Ser142	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.8 \cdot 10^{4}$	$2.3 \cdot 10^{-6} < K_{op} < 3.4 \cdot 10^{-3}$	$3.5 < \Delta G_{op} < 8.0$
Arg143	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.2 \cdot 10^{4}$	$3.3 \cdot 10^{-6} < K_{op} < 4.9 \cdot 10^{-3}$	$3.3 < \Delta G_{op} < 7.8$
Leu144	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$2.2 \cdot 10^{3}$	$< 1.6 \cdot 10^{-9}$	> 12.5
Ala145	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$3.1 \cdot 10^{3}$	$< 1.2 \cdot 10^{-8}$	> 11.2
Cys146	$2.8 \cdot 10^{-3}$	$2.5 \cdot 10^{2}$	$2.1 \cdot 10^{4}$	$1.3 \cdot 10^{-7}$	9.8
Gly147	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$3.4 \cdot 10^{4}$	$< 1.1 \cdot 10^{-9}$	> 12.7
Val148	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.5 \cdot 10^{3}$	$2.7 \cdot 10^{-5} < K_{op} < 4.0 \cdot 10^{-2}$	$2.0 < \Delta G_{op} < 6.5$
Ile149	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$6.9 \cdot 10^{2}$	$< 5.2 \cdot 10^{-8}$	> 10.3
Gly150	$< 3.6 \cdot 10^{-5}$	$> 1.9 \cdot 10^{4}$	$5.6 \cdot 10^{3}$	$< 6.4 \cdot 10^{-9}$	> 11.5
Ile151	n/a	n/a	n/a	n/a	n/a
Ala152	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$3.0 \cdot 10^{3}$	$1.3 \cdot 10^{-5} < K_{op} < 2.0 \cdot 10^{-2}$	$2.4 < \Delta G_{op} < 6.9$
Gln153	$3.4 \cdot 10^{-4}$	$2.1 \cdot 10^{3}$	$5.8 \cdot 10^{3}$	$5.8 \cdot 10^{-8}$	10.3

Table 2: Supplementary Table 2: H/D exchange parameters for I113T at 25°C

Residue	$k_{ex}(min^{-1})$	$t_{1/2}(min)$	$k_{ch}(min^{-1})$	K_{op}	$\Delta G_{op}(kcalmol^{-1}l^{-1})$
Ala1	n/a	n/a	n/a	n/a	n/a
Thr2	n/a	n/a	n/a	n/a	n/a
Lys3	n/a	n/a	n/a	n/a	n/a
Ala4	$8.8 \cdot 10^{-3}$	$7.9 \cdot 10^{1}$	$7.0 \cdot 10^{4}$	$1.3 \cdot 10^{-7}$	9.8
Val5	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$3.3 \cdot 10^{2}$	$< 1.7 \cdot 10^{-7}$	> 9.6
Cys6	$7.9 \cdot 10^{-5}$	$8.7 \cdot 10^{3}$	$1.2 \cdot 10^{3}$	$6.6 \cdot 10^{-8}$	10.2
Val7	n/a	n/a	n/a	n/a	n/a
Leu8	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$4.4 \cdot 10^{2}$	$< 1.1 \cdot 10^{-7}$	> 10.6
Lys9	$9.3 \cdot 10^{-5}$	$7.5 \cdot 10^{3}$	$9.4 \cdot 10^{2}$	$9.9 \cdot 10^{-8}$	9.9
Gly10	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$4.1 \cdot 10^{3}$	$9.8 \cdot 10^{-6} < K_{op} < 1.5 \cdot 10^{-2}$	$2.6 < \Delta G_{op} < 7.1$
Asp11	$7.7 \cdot 10^{1}$	$8.9 \cdot 10^{-3}$	$1.2 \cdot 10^{3}$	$6.3 \cdot 10^{-2}$	1.7
Gly12	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$2.1 \cdot 10^{3}$	$1.9 \cdot 10^{-5} < K_{op} < 2.9 \cdot 10^{-5}$	$2.2 < \Delta G_{op} < 6.7$
Pro13	n/a	n/a	n/a	n/a	n/a
Val14	$1.4 \cdot 10^{-4}$	$5.0 \cdot 10^{3}$	$4.9 \cdot 10^{2}$	$2.8 \cdot 10^{-7}$	9.3
Gln15	$3.1 \cdot 10^{-2}$	$2.2 \cdot 10^{1}$	$1.4 \cdot 10^{3}$	$2.2 \cdot 10^{-5}$	6.6
Gly16	$3.6 \cdot 10^{-4}$	$1.9 \cdot 10^{3}$	$4.6 \cdot 10^{3}$	$7.8 \cdot 10^{-8}$	10.1
Val17	$7.8 \cdot 10^{-4}$	$8.9 \cdot 10^{2}$	$4.6 \cdot 10^{2}$	$1.7 \cdot 10^{-6}$	8.2
Ile18	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$1.8 \cdot 10^{2}$	$< 3.7 \cdot 10^{-7}$	> 9.1
Asn19	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$3.0 \cdot 10^{3}$	$< 2.2 \cdot 10^{-8}$	> 10.8
Phe20	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$2.0 \cdot 10^{3}$	$< 3.3 \cdot 10^{-8}$	> 10.6
Glu21	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$5.9 \cdot 10^{2}$	$< 1.1 \cdot 10^{-7}$	> 9.9
Gln22	$2.0 \cdot 10^{-4}$	$3.5 \cdot 10^{3}$	$1.4 \cdot 10^{3}$	$1.4 \cdot 10^{-7}$	9.7
Lys23	n/a	n/a	$2.4 \cdot 10^{3}$	n/a	n/a
Glu24	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$6.8 \cdot 10^{2}$	$5.9 \cdot 10^{-5} < K_{op} < 8.8 \cdot 10^{-2}$	$1.5 < \Delta G_{op} < 6.0$
Ser25	n/a	n/a	n/a	n/a	n/a
Asn26	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$1.0 \cdot 10^{4}$	$< 7.0 \cdot 10^{-9}$	> 11.4
Gly27	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$6.5 \cdot 10^{3}$	$6.2 \cdot 10^{-6} < K_{op} < 9.2 \cdot 10^{-3}$	$2.9 < \Delta G_{op} < 7.4$
Pro28	n/a	n/a	n/a	n/a	n/a
Val29	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$1.3 \cdot 10^{3}$	$< 5.1 \cdot 10^{-8}$	> 10.3
Lys30	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$1.1 \cdot 10^{3}$	$< 5.2 \cdot 10^{-8}$	> 10.2
Val31	$7.7 \cdot 10^{-5}$	$9.0 \cdot 10^{3}$	$4.4 \cdot 10^{2}$	$1.7 \cdot 10^{-7}$	9.6
Trp32	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$4.7 \cdot 10^{2}$	$< 1.4 \cdot 10^{-7}$	> 9.7
Gly33	$6.7 \cdot 10^{-5}$	$1.0 \cdot 10^{4}$	$2.4 \cdot 10^{3}$	$2.8 \cdot 10^{-8}$	10.8
Ser34	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$5.8 \cdot 10^{3}$	$6.9 \cdot 10^{-6} < K_{op} < 1.0 \cdot 10^{-2}$	$2.8 < \Delta G_{op} < 7.3$
Ile35	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$6.2 \cdot 10^{2}$	$< 1.1 \cdot 10^{-7}$	> 9.9
Lys36	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$9.0 \cdot 10^{2}$	$< 7.3 \cdot 10^{-8}$	> 10.1
Gly37	$3.2 \cdot 10^{-3}$	$2.2 \cdot 10^{2}$	$4.1 \cdot 10^{3}$	$7.7 \cdot 10^{-7}$	8.7
Leu38	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$6.5 \cdot 10^{2}$	$< 1.0 \cdot 10^{-7}$	> 9.9
Thr39	$< 6.6 \cdot 10^{-5}$	$9.9 \cdot 10^{3}$	$8.8 \cdot 10^{2}$	$< 8.0 \cdot 10^{-8}$	> 10.1
Glu40	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$8.2 \cdot 10^{2}$	$< 8.0 \cdot 10^{-8}$	> 10.1
Gly41	$4.6 \cdot 10^{-4}$	$1.5 \cdot 10^{3}$	$2.2 \cdot 10^{3}$	$2.1 \cdot 10^{-7}$	9.5
Leu42	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$6.5 \cdot 10^{2}$	$< 1.1 \cdot 10^{-8}$	> 11.3
His43	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$6.5 \cdot 10^{3}$	$< 1.1 \cdot 10^{-9}$	> 12.7
Gly44	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$2.1 \cdot 10^{4}$	$< 1.0 \cdot 10^{-9}$	> 12.7
Phe45	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$1.4 \cdot 10^{3}$	$< 1.0 \cdot 10^{-8}$	> 11.3
His46	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$1.2 \cdot 10^{4}$	$< 5.5 \cdot 10^{-9}$	> 11.8
Val47	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$3.8 \cdot 10^{3}$	$< 1.6 \cdot 10^{-8}$	> 11.0
His48	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$7.6 \cdot 10^{3}$	$5.2 \cdot 10^{-6} < K_{op} < 7.9 \cdot 10^{-3}$	$3.0 < \Delta G_{op} < 7.5$
Glu49	$1.5 \cdot 10^{2}$	$4.1 \cdot 10^{-3}$	$3.5 \cdot 10^{3}$	$4.2 \cdot 10^{-2}$	2.0
Phe50	$6.9 \cdot 10^{1}$	$1.0 \cdot 10^{-2}$	$6.8 \cdot 10^{2}$	$1.0 \cdot 10^{-1}$	1.4
Gly51	$8.5 \cdot 10^{-4}$	$8.2 \cdot 10^{2}$	$3.6 \cdot 10^{3}$	$2.4 \cdot 10^{-7}$	9.4
Asp52	$8.6 \cdot 10^{-4}$	$8.1 \cdot 10^{2}$	$1.2 \cdot 10^{3}$	$7.0 \cdot 10^{-7}$	8.7
Asn53	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}1$	$3.4 \cdot 10^{3}$	$< 1.9 \cdot 10^{-8}$	> 10.9
Thr54	$5.2 \cdot 10^{-3}$	$1.3 \cdot 10^{2}$	$3.0 \cdot 10^{3}$	$1.7 \cdot 10^{-6}$	8.2
Ala55	$1.5 \cdot 10^{2}$	$4.7 \cdot 10^{-3}$	$2.6 \cdot 10^{3}$	$5.6 \cdot 10^{-2}$	1.8
Gly56	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$3.1 \cdot 10^{3}$	$1.3 \cdot 10^{-5} < K_{op} < 1.9 \cdot 10^{-2}$	$2.4 < \Delta G_{op} < 6.9$
Cys57	n/a	n/a	n/a	n/a	n/a
Thr58	n/a	n/a	n/a	n/a	n/a
Ser59	$1.0 \cdot 10^{2}$	$6.8 \cdot 10^{-3}$	$6.2 \cdot 10^{3}$	$1.6 \cdot 10^{-2}$	2.5
Ala60	$1.0 \cdot 10^{-3}$	$6.8 \cdot 10^{2}$	$3.3 \cdot 10^{3}$	$3.0 \cdot 10^{-7}$	9.2
Gly61	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$3.1 \cdot 10^{3}$	$1.3 \cdot 10^{-5} < K_{op} < 1.9 \cdot 10^{-2}$	$2.4 < \Delta G_{op} < 6.9$

Residue	$k_{ex}(min^{-1})$	$t_{1/2}(min)$	$k_{ch}(min^{-1})$	K_{op}	$\Delta G_{op}(kcalmol^{-1}l^{-1})$
Pro62	n/a	n/a	n/a	n/a	n/a
His63	$3.7 \cdot 10^{-2}$	$1.9 \cdot 10^{1}$	$1.6 \cdot 10^{4}$	$2.4 \cdot 10^{-6}$	8.0
Phe64	n/a	n/a	$6.5 \cdot 10^{3}$	n/a	n/a
Asn65	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$5.9 \cdot 10^{3}$	$6.7 \cdot 10^{-6} < K_{op} < 1.0 \cdot 10^{-2}$	$2.8 < \Delta G_{op} < 7.3$
Pro66	n/a	n/a	n/a	n/a	n/a
Leu67	$4.2 \cdot 10^{2}$	$1.6 \cdot 10^{-3}$	$1.8 \cdot 10^{3}$	$2.4 \cdot 10^{-1}$	0.9
Ser68	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$2.4 \cdot 10^{3}$	$1.7 \cdot 10^{-5} < K_{op} < 2.5 \cdot 10^{-2}$	$2.5 < \Delta G_{op} < 7.5$
Arg69	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$4.0 \cdot 10^{3}$	$1.0 \cdot 10^{-5} < K_{op} < 1.5 \cdot 10^{-2}$	$2.6 < \Delta G_{op} < 7.1$
Lys70	$1.0 \cdot 10^{2}$	$6.7 \cdot 10^{-3}$	$2.5 \cdot 10^{3}$	$4.1 \cdot 10^{-2}$	2.0
His71	$2.0 \cdot 10^{-4}$	$3.4 \cdot 10^{3}$	$1.4 \cdot 10^{4}$	$1.5 \cdot 10^{-8}$	11.1
Gly72	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$2.1 \cdot 10^{4}$	$< 3.0 \cdot 10^{-9}$	> 12.1
Gly73	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$4.6 \cdot 10^{3}$	$< 1.4 \cdot 10^{-8}$	> 11.1
Pro74	n/a	n/a	n/a	n/a	n/a
Lys75	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$6.1 \cdot 10^{3}$	$6.6 \cdot 10^{-6} < K_{op} < 9.9 \cdot 10^{-3}$	$2.8 < \Delta G_{op} < 7.3$
Asp76	$3.5 \cdot 10^{-3}$	$2.0 \cdot 10^{2}$	$1.1 \cdot 10^{3}$	$3.1 \cdot 10^{-6}$	7.8
Glu77	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$3.4 \cdot 10^{2}$	$1.1 \cdot 10^{-4} < K_{op} < 1.8 \cdot 10^{-1}$	$1.1 < \Delta G_{op} < 5.6$
Glu78	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$3.6 \cdot 10^{2}$	$1.9 \cdot 10^{-4} < K_{op} < 1.4 \cdot 10^{-1}$	$1.1 < \Delta G_{op} < 5.6$
Arg79	$1.3 \cdot 10^{-3}$	$5.3 \cdot 10^{2}$	$1.4 \cdot 10^{3}$	$9.2 \cdot 10^{-7}$	8.6
His80	$7.4 \cdot 10^{1}$	$9.4 \cdot 10^{-3}$	$1.8 \cdot 10^{4}$	$4.2 \cdot 10^{-3}$	3.4
Val81	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$2.2 \cdot 10^{3}$	$1.8 \cdot 10^{-5} < K_{op} < 2.7 \cdot 10^{-2}$	$2.2 < \Delta G_{op} < 6.7$
Gly82	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$2.6 \cdot 10^{3}$	$1.5 \cdot 10^{-5} < K_{op} < 2.2 \cdot 10^{-2}$	$2.4 < \Delta G_{op} < 6.8$
Asp83	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$1.2 \cdot 10^{3}$	$< 5.5 \cdot 10^{-8}$	> 10.3
Leu84	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$2.9 \cdot 10^{2}$	$< 2.3 \cdot 10^{-7}$	> 9.4
Gly85	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$1.9 \cdot 10^{3}$	$< 3.5 \cdot 10^{-8}$	> 10.6
Asn86	$3.1 \cdot 10^{-4}$	$2.2 \cdot 10^{3}$	$7.6 \cdot 10^{3}$	$4.1 \cdot 10^{-8}$	10.5
Val87	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$7.0 \cdot 10^{2}$	$< 9.4 \cdot 10^{-8}$	> 10.0
Thr88	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.0 \cdot 10^{3}$	$3.9 \cdot 10^{-5} < K_{op} < 5.8 \cdot 10^{-2}$	$1.8 < \Delta G_{op} < 6.2$
Ala89	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$2.6 \cdot 10^{3}$	$< 2.5 \cdot 10^{-8}$	> 10.8
Asp90	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$8.4 \cdot 10^{2}$	$4.8 \cdot 10^{-5} < K_{op} < 7.2 \cdot 10^{-2}$	$1.6 < \Delta G_{op} < 6.1$
Lys91	$8.5 \cdot 10^{1}$	$8.2 \cdot 10^{-3}$	$1.0 \cdot 10^{3}$	$8.4 \cdot 10^{-2}$	1.5
Asp92	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$1.1 \cdot 10^{3}$	$3.6 \cdot 10^{-5} < K_{op} < 5.4 \cdot 10^{-2}$	$1.8 < \Delta G_{op} < 6.3$
Gly93	$5.5 \cdot 10^{-4}$	$1.3 \cdot 10^{3}$	$2.1 \cdot 10^{3}$	$2.7 \cdot 10^{-7}$	9.3
Val94	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$4.9 \cdot 10^{2}$	$< 1.4 \cdot 10^{-7}$	> 9.7
Ala95	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$1.2 \cdot 10^{3}$	$< 5.5 \cdot 10^{-8}$	> 10.3
Asp96	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$8.4 \cdot 10^{2}$	$4.8 \cdot 10^{-5} < K_{op} < 7.2 \cdot 10^{-2}$	$1.6 < \Delta G_{op} < 6.1$
Val97	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$2.2 \cdot 10^{2}$	$< 3.0 \cdot 10^{-7}$	> 9.2
Ser98	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$2.8 \cdot 10^{3}$	$1.4 \cdot 10^{-5} < K_{op} < 2.1 \cdot 10^{-2}$	$2.4 < \Delta G_{op} < 6.9$
Ile99	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$6.2 \cdot 10^{2}$	$< 1.1 \cdot 10^{-7}$	> 9.9
Glu100	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$3.0 \cdot 10^{2}$	$< 2.2 \cdot 10^{-7}$	> 9.4
Asp101	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$2.8 \cdot 10^{3}$	$1.4 \cdot 10^{-5} < K_{op} < 2.1 \cdot 10^{-2}$	$2.4 < \Delta G_{op} < 6.9$
Ser102	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$7.9 \cdot 10^{3}$	$5.1 \cdot 10^{-6} < K_{op} < 7.6 \cdot 10^{-3}$	$3.0 < \Delta G_{op} < 7.5$
Val103	n/a	n/a	n/a	n/a	n/a
Ile104	n/a	n/a	n/a	n/a	n/a
Ser105	n/a	n/a	n/a	n/a	n/a
Leu106	n/a	n/a	n/a	n/a	n/a
Ser107	n/a	n/a	n/a	n/a	n/a
Gly108	n/a	n/a	n/a	n/a	n/a
Asp109	n/a	n/a	n/a	n/a	n/a
His110	n/a	n/a	n/a	n/a	n/a
Cys111	n/a	n/a	n/a	n/a	n/a
Ile112	n/a	n/a	n/a	n/a	n/a
Thr113	n/a	n/a	n/a	n/a	n/a
Gly114	n/a	n/a	n/a	n/a	n/a
Arg115	$8.6 \cdot 10^{-4}$	$8.1 \cdot 10^{2}$	$4.0 \cdot 10^{3}$	$2.1 \cdot 10^{-7}$	9.5
Thr116	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$2.4 \cdot 10^{3}$	$< 2.8 \cdot 10^{-8}$	> 10.7
Leu117	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$7.0 \cdot 10^{2}$	$< 9.4 \cdot 10^{-8}$	> 10.0
Val118	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$2.0 \cdot 10^{2}$	$< 3.3 \cdot 10^{-7}$	> 9.2
Val119	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$2.4 \cdot 10^{2}$	$< 2.8 \cdot 10^{-7}$	> 9.3
His120	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$7.6 \cdot 10^{3}$	$< 9.0 \cdot 10^{-9}$	> 11.4
Glu121	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$3.5 \cdot 10^{3}$	$< 1.9 \cdot 10^{-8}$	> 10.9
Lys122	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$1.1 \cdot 10^{3}$	$< 6.0 \cdot 10^{-8}$	> 10.2
Ala123	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$2.2 \cdot 10^{3}$	$1.8 \cdot 10^{-5} < K_{op} < 2.7 \cdot 10^{-2}$	$2.2 < \Delta G_{op} < 6.7$
Asp124	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$8.4 \cdot 10^{2}$	$< 7.9 \cdot 10^{-8}$	> 10.1
Asp125	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$5.5 \cdot 10^{2}$	$< 1.2 \cdot 10^{-7}$	> 9.9
Leu126	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$2.9 \cdot 10^{2}$	$< 2.3 \cdot 10^{-7}$	> 9.4

Residue	$k_{ex}(min^{-1})$	$t_{1/2}(min)$	$k_{ch}(min^{-1})$	K_{op}	$\Delta G_{op}(kcalmol^{-1}l^{-1})$
Gly127	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$1.9 \cdot 10^{3}$	$3.4 \cdot 10^{-9}$	12.0
Lys128	$3.3 \cdot 10^{-4}$	$2.1 \cdot 10^{3}$	$2.3 \cdot 10^{3}$	$1.5 \cdot 10^{-7}$	9.7
Gly129	$1.5 \cdot 10^{2}$	$4.7 \cdot 10^{-3}$	$4.1 \cdot 10^{3}$	$3.6 \cdot 10^{-2}$	2.1
Gly130	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$4.6 \cdot 10^{3}$	$8.7 \cdot 10^{-6} < K_{op} < 1.3 \cdot 10^{-2}$	$2.7 < \Delta G_{op} < 7.2$
Asn131	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$7.6 \cdot 10^{3}$	$5.2 \cdot 10^{-6} < K_{op} < 7.9 \cdot 10^{-3}$	$3.0 < \Delta G_{op} < 7.5$
Glu132	n/a	n/a	n/a	n/a	n/a
Glu133	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$3.6 \cdot 10^{2}$	$1.1 \cdot 10^{-4} < K_{op} < 1.6 \cdot 10^{-1}$	$1.1 < \Delta G_{op} < 5.6$
Ser134	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$2.8 \cdot 10^{3}$	$1.4 \cdot 10^{-5} < K_{op} < 2.2 \cdot 10^{-2}$	$2.4 < \Delta G_{op} < 6.9$
Thr135	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$2.8 \cdot 10^{3}$	$1.4 \cdot 10^{-5} < K_{op} < 2.1 \cdot 10^{-2}$	$2.4 < \Delta G_{op} < 6.9$
Lys136	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$2.4 \cdot 10^{3}$	$1.7 \cdot 10^{-5} < K_{op} < 2.5 \cdot 10^{-2}$	$2.3 < \Delta G_{op} < 6.8$
Thr137	$8.0 \cdot 10^{1}$	$8.6 \cdot 10^{-3}$	$1.9 \cdot 10^{3}$	$4.3 \cdot 10^{-2}$	1.9
Gly138	$5.0 \cdot 10^{-4}$	$1.4 \cdot 10^{3}$	$4.9 \cdot 10^{3}$	$1.0 \cdot 10^{-7}$	9.9
Asn139	$7.3 \cdot 10^{-4}$	$9.5 \cdot 10^{2}$	$7.6 \cdot 10^{3}$	$9.6 \cdot 10^{-8}$	10.0
Ala140	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$3.5 \cdot 10^{3}$	$1.2 \cdot 10^{-5} < K_{op} < 1.7 \cdot 10^{-2}$	$2.5 < \Delta G_{op} < 7.0$
Gly141	$7.9 \cdot 10^{1}$	$8.6 \cdot 10^{-3}$	$3.1 \cdot 10^{3}$	$2.5 \cdot 10^{-2}$	2.3
Ser142	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$5.8 \cdot 10^{3}$	$6.9 \cdot 10^{-6} < K_{op} < 1.0 \cdot 10^{-2}$	$2.8 < \Delta G_{op} < 7.3$
Arg143	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$4.0 \cdot 10^{3}$	$1.0 \cdot 10^{-5} < K_{op} < 1.5 \cdot 10^{-2}$	$2.6 < \Delta G_{op} < 7.1$
Leu144	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$7.2 \cdot 10^{2}$	$< 9.2 \cdot 10^{-8}$	> 10.0
Ala145	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$1.1 \cdot 10^{3}$	$< 6.0 \cdot 10^{-8}$	> 10.2
Cys146	$3.8 \cdot 10^{-4}$	$1.8 \cdot 10^{3}$	$7.0 \cdot 10^{3}$	$5.4 \cdot 10^{-8}$	10.3
Gly147	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$1.1 \cdot 10^{4}$	$< 6.0 \cdot 10^{-9}$	> 11.7
Val148	$2.1 \cdot 10^{-3}$	$2.4 \cdot 10^{2}$	$4.9 \cdot 10^{2}$	$4.2 \cdot 10^{-6}$	7.6
Ile149	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$2.2 \cdot 10^{2}$	$< 3.0 \cdot 10^{-7}$	> 9.3
Gly150	$< 6.6 \cdot 10^{-5}$	$> 1.0 \cdot 10^{4}$	$1.8 \cdot 10^{3}$	$< 3.7 \cdot 10^{-8}$	> 10.5
Ile151	n/a	n/a	n/a	n/a	n/a
Ala152	$4 \cdot 10^{-2} < k_{ex} < 6 \cdot 10^{1}$	$1.2 \cdot 10^{-2} < t_{1/2} < 1.7 \cdot 10^{1}$	$9.8 \cdot 10^{2}$	$4.1 \cdot 10^{-5} < K_{op} < 6.1 \cdot 10^{-2}$	$1.7 < \Delta G_{op} < 6.2$
Gln153	$8.9 \cdot 10^{-5}$	$7.7 \cdot 10^{3}$	$1.9 \cdot 10^{3}$	$4.7 \cdot 10^{-8}$	10.4